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REPORT DOCUMENTATION PAC

1a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED			1b. RES		
2a. SECURITY CLASSIFICATION AUTHORITY			3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution is unlimited.		
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE			5. MONITORING ORGANIZATION REPORT NUMBER(S) AFOSR-TR- 92 0797		
4. PERFORMING ORGANIZATION REPORT NUMBER(S)		7a. NAME OF MONITORING ORGANIZATION AFOSR/NE/L			
6a. NAME OF PERFORMING ORGANIZATION (EXAMPLE) North Carolina Central University		6b. OFFICE SYMBOL (if applicable) NE/L		7b. ADDRESS (City, State, and ZIP Code) Building 410, Bolling AFB DC 20332-6448	
6c. ADDRESS (City, State, and ZIP Code)		9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER Grant/Contract Number F49620-89-C-0080			
8a. NAME OF FUNDING/SPONSORING ORGANIZATION AFOSR		8b. OFFICE SYMBOL (if applicable) NE/L		10. SOURCE OF FUNDING NUMBERS	
8c. ADDRESS (City, State, and ZIP Code) Building 410, Bolling AFB DC 20332-6448		PROGRAM ELEMENT NO. 61102F		PROJECT NO. 2310	TASK NO. A2
11. TITLE (Include Security Classification) High Resolution Molecular Spectroscopy of Atmospheric Species					
12. PERSONAL AUTHOR(S) Drs. Jyotsna M. Dutta and Charles R. Jones Author(s) on Reprint, Interim or Final Report					
13a. TYPE OF REPORT Final Annual		13b. TIME COVERED FROM 7-1-91 TO 6-30-92		14. DATE OF REPORT (Year, Month, Day)	
15. PAGE COUNT					
16. SUPPLEMENTARY NOTATION (Journal Citation) - Name of Journal, Volume Number, Page Numbers, data. (USE WITH REPRINTS ONLY)					
17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)		
FIELD	GROUP	SUB-GROUP			
19. ABSTRACT (Continue on reverse if necessary and identify by block number) The pressure-broadening of the 2(1,1) - 2(1,2), 3(1,3) - 2(2,1), and 7(3,4) - 6(4,3) transitions of HDO were studied between 90K and 600K. The broadening gases were He, H ₂ , O ₂ , and N ₂ . Results for the temperature dependence of the pressure broadening parameters and collisional cross sections are discussed. The HDO transitions selected for study belong to widely different lower state energies. Such a selection allows to observe any dependence that 300K broadening parameters and temperature coefficients may have on the rotational quantum numbers. All these have considerable theoretical interest.					
20. DISTRIBUTION/AVAILABILITY OF ABSTRACT <input checked="" type="checkbox"/> UNCLASSIFIED/UNLIMITED <input type="checkbox"/> SAME AS RPT. <input type="checkbox"/> DTIC USERS					
21. ABSTRACT SECURITY CLASSIFICATION UNCLASSIFIED					
22a. NAME OF RESPONSIBLE INDIVIDUAL James G. Stobie Program Manager		22b. TELEPHONE (Include Area Code) (202) 767-4968		22c. OFFICE SYMBOL AFOSR/NE/L	

92-22989



2 8 18 040

Title: High Resolution Molecular Spectroscopy of Atmospheric Species

Contract/Grant Number: F49620-89-C-0080

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Reporting Period: July 1, 1991 to June 30, 1992.

Research Participants: Mr. Ralph France, III

Summary of Objectives and Accomplishments

1. Pressure broadening measurements were performed on the $3(1,2) - 2(2,1)$, $2(1,1) - 2(1,2)$, and $7(3,4) - 6(4,3)$ transitions of HDO at 225,896.72 MHz, 241,562 MHz, and 241974 MHz respectively. Broadening gases were He, H₂, O₂ and N₂. Temperature dependence of the pressure broadening parameters were studied between 90K and 600K.
2. Results of the research were presented at various scientific meetings during this reporting period. These meetings are:
 - i) 16th International Conference on IR and MM Waves, Lausanne, Switzerland, 26-30 August 1991. Conference Digest pp.
 - ii) South Eastern Section Meeting of the American Physical Society, Nov. 11-13, 1991. Bull. Am. Phys. Soc. V. 36, #10, p. 2731, Nov. 1991. iii) American Physical Society March Meeting. Indianapolis, March 16-20, 1992. Bull. Am. Phys. Soc., 37, 520 (1992).
 - iv) International Symposium on Molecular Spectroscopy, June 15-10, 1992, Columbus, Ohio.
3. Mr. Ralph France, III, a research participant has completed his B.S. program. He presented a paper at the 6th National Undergraduate Research Meeting, Minneapolis, March 25-29, 1992, describing his research for the project.

ABSTRACT

The pressure-broadening of the $2(1,1) - 2(1,2)$, $3(1,2) - 2(2,1)$, and $7(3,4) - 6(4,3)$ transitions of HDO were studied between 90K and 600K. The broadening gases were He, H_2 , O_2 , and N_2 . Results for the temperature dependence of the pressure broadening parameters and collisional cross sections are discussed. The HDO transitions selected for study belong to widely different lower state energies. Such a selection allows to observe any dependence that 300K broadening parameters and temperature coefficients may have on the rotational quantum numbers. All these have considerable theoretical interest.

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HDO is a prolate asymmetric rotor with both "a" and b transitions. Because of the small moments of inertia and large rotational constants, microwave spectra are very sparse. The presence of HDO has been detected in the upper atmosphere as well as in the interstellar medium.

Pressure-broadening measurements were performed on 2(1,1) - 2(1,2), 3(1,2) - 2(2,1), and 7(3,4) - 6(4,3) transitions at 241561.55 MHz, and 225896.72, and 241973.57 MHz respectively. The corresponding energy values of the lower levels are 58.1269 cm⁻¹, 108.9262 cm⁻¹, and 573.890 cm⁻¹ (1). The rotational lines were selected for the measurements to study the temperature dependence of their pressure broadening coefficients and pressure broadening cross sections. Lines with a wide range of energies and J values were deliberately chosen because of their potential theoretical implications.

Broadband spectrometer used for the measurement has been shown in Fig. 1. Low temperature measurements were made in a collisionally cooled cell with a continuously variable temperature between 80K and 300K. Usable upper temperature limit is set by the trapping point of the sample gas (Fig. 2). Static measurements were made in a quartz cell enclosed in an oven with a continuously variable temperature between 80K and 600K. The broadening gases used were He, H₂, O₂, and N₂.

The pressure of the broadening gas is typically varied from 0.02 to 1.0 torr. For each temperature, data were recorded for about 30 different pressures. Each line profile was fit to the voight line shape to extract the halfwidth ($\Delta\nu$). Pressure-broadening coefficient γ , for each temperature was obtained from a least square fit to the data, using the relation

$$\Delta\nu = \gamma P \quad (1)$$

Pressure broadening parameters as well as collisional parameters are strong functions of temperature. It has been found that observed pressure broadening data can accurately be represented by

$$\sigma(T) = \sigma_0(T_0/T)^m \quad (2)$$

$$\text{and} \quad \gamma(T) = \gamma_0(T_0/T)^n \quad (3)$$

where σ_0 and γ_0 are the cross section and pressure broadening parameters at the reference temperature T_0 , respectively, n and m are constants.

Fig. 3 shows the experimental results for HDO-He collisions. Data followed equation (3) and fall on a straight line. As can be seen in Fig. 3, the helium data for all three lines show no significant deviation from the straight lines. N values are shown in Table 1 and these are close to 0.5, a result predicted by hard sphere collision theory. It may be noted that helium does not possess any multipole moment and these are results which are expected.

HDO lines broadened by H_2 is shown in Fig. 4. High temperature data, up to 150K, followed Eqn. (3) and fall on straight lines with the values of the slopes which are shown in Table 1. Low temperature data have considerable deviation from the straight line. Similar fall-off of the low temperature data has been observed for these lines broadened by O_2 and N_2 and shown in Figs. 5 and 6 respectively. High temperature data, up to 150K, followed Eqn. (3) and fall on straight lines with the values of the slopes which are shown in Table 1. The pressure broadening cross sections are calculated via the relation

$$\sigma = 0.447 (\mu T)^{1/2} \gamma ; \quad (4)$$

where $\sigma(A^2)$ is the pressure broadening cross sections, $\mu(\text{amu})$ the reduced mass, $T(K)$ the temperature, and $\gamma(\text{MHz/Torr})$ the pressure broadening parameter. The collisional cross sections for three transitions of HDO with H_2 , He, O_2 , and N_2 at temperatures between 80K and 600K are shown in Figs. 7-9. Here again, we find that helium data follow Eqn (2) with $m = 0$ and fall on straight lines which are parallel to Temperature-axis, showing that these represent hard sphere scattering. High temperature data for the $2(1,1) - 2(1,2)$ and $3(1,2) - 2(2,1)$ transitions broadened by H_2 , O_2 , and N_2 follow Eq. (2). However, the low temperature data (below 150K) show considerable drop of their values. Fig.10 shows the broadening parameters as a function of J . We notice a trend for all of these four broadening gases - decrease in the broadening coefficients for increase in J values. The broadening parameters for collision with nitrogen are larger than with other molecules considered here. It can be accounted for the by the fact that nitrogen has the largest value for quadrupole moment compared to other broadening gases studied. Fig. 10 also shows HDO - N_2 broadening results due to Devi et al (2). Their measured values are within our experimental errors and their values also show a trend similar to ours.

Fig. 11 plots the temperature exponent, n versus J for the broadening gases. He - data show no variation with respect to J . Only in the case of hydrogen broadening data we notice a definite trend -decrease in n value with increase in J . Same conclusion cannot be drawn for the oxygen and nitrogen-broadening data.

CONCLUSION

Experimental studies reported here include pressure broadening measurements of several HDO lines broadened by H_2 , He, N_2 , and O_2 over a large temperature range. Availability of a dependable theoretical framework would facilitate interpolation and extrapolation of measured values as a function of both temperature and quantum number. However, the calculation of pressure broadening parameter is a very complicated problem. Clearly it is important to develop a reliable body of experimental data bank for various molecular species of atmospheric importance. An effort reported here would contribute to develop such a data bank.

REFERENCES

1. J. K. Messer, Frank C. DeLucia, and Paul Helminger, *J. of Mole. Spectrosc.* 105, 139-155 (1984).
2. V. Malathy Devi, D. C. Benner, C. P. Rinsland, M. A. H. Smith, and B. D. Sidney, *J. Mole. Spectrosc.* 117, 403 (1986).

Table of results for HDO pressure broadening
(γ in MHz/torr)

		$2_{1,1}-2_{1,2}$	$3_{1,2}-2_{2,1}$	$7_{3,4}-6_{4,3}$
Helium	n	0.50(5)	0.52(3)	0.50(5)
	γ_0	0.784(1)	0.74(1)	0.52(1)
Hydrogen	n	0.86(5)	0.81(2)	0.59(3)
	γ_0	3.9(1)	3.48(3)	2.51(4)
Oxygen	n	0.90(3)	0.96(2)	0.81(6)
	γ_0	2.71(5)	2.25(2)	1.58(5)
Nitrogen	n	0.77(1)	0.70(2)	0.67(5)
	γ_0	4.45(6)	4.21(4)	3.47(6)

Table 1.

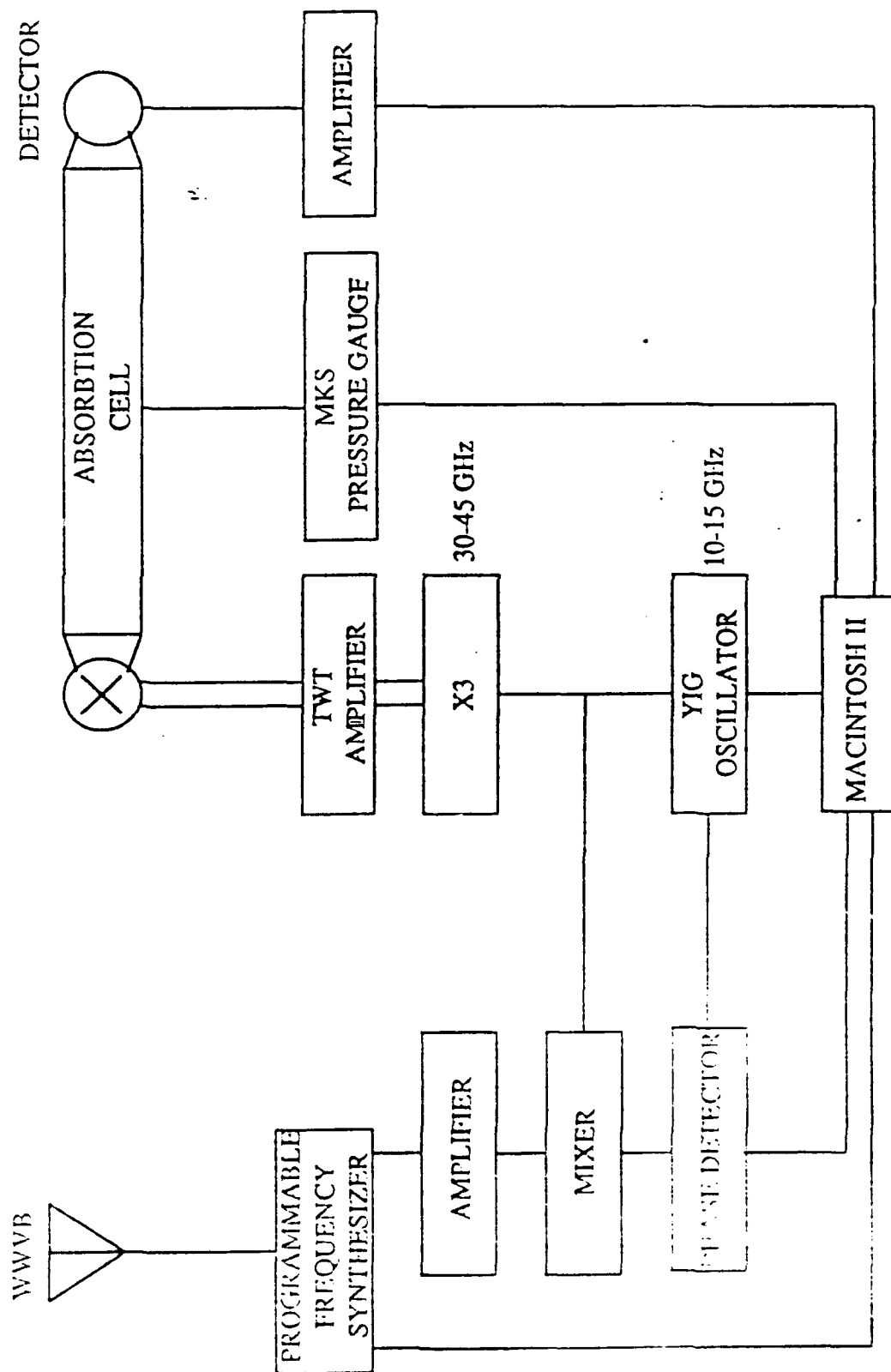


Fig. 1 Broadband Spectrometer

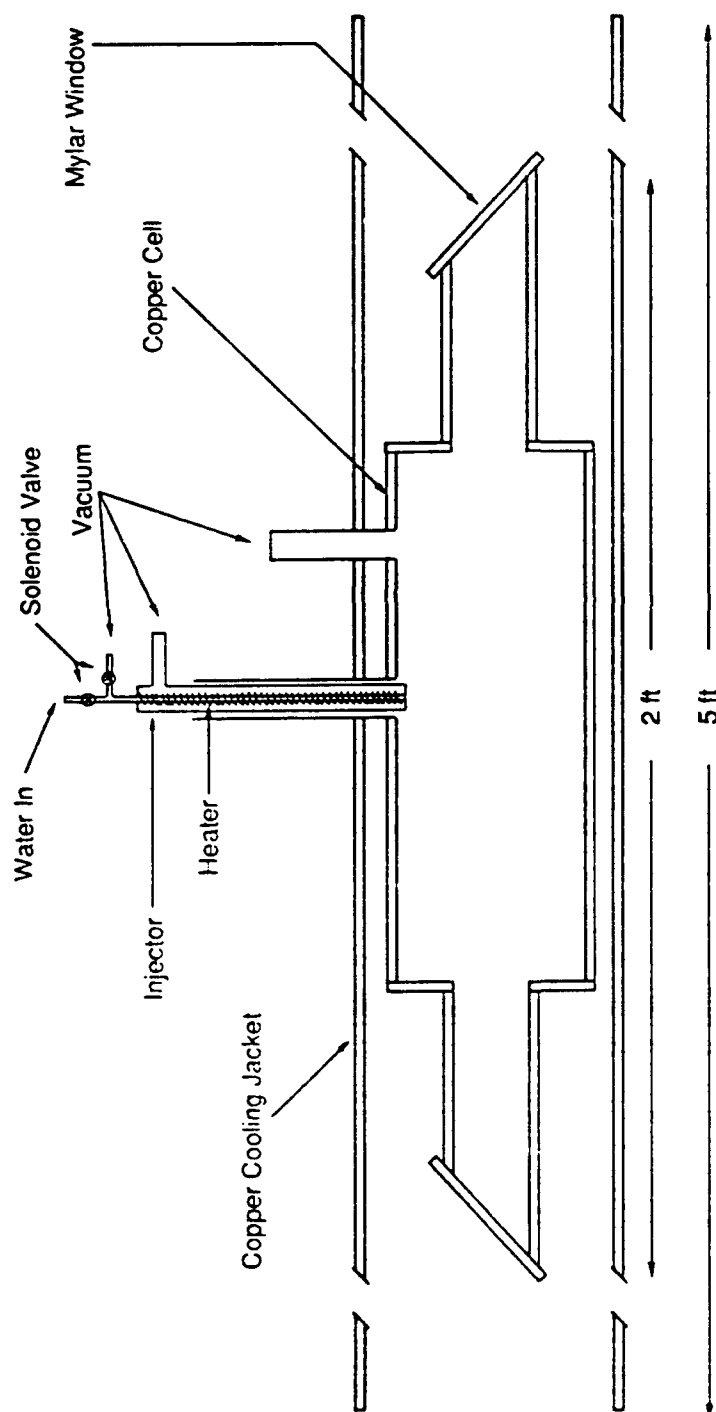


Fig. 2 Collisionally Cooled Cell

HDO-Helium Broadening

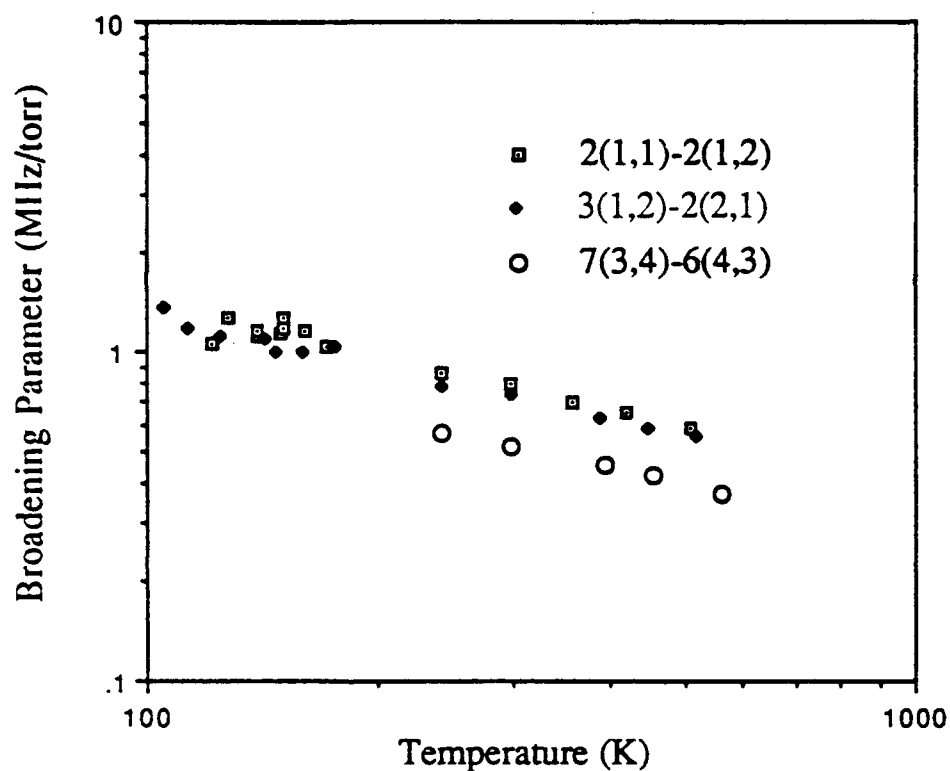
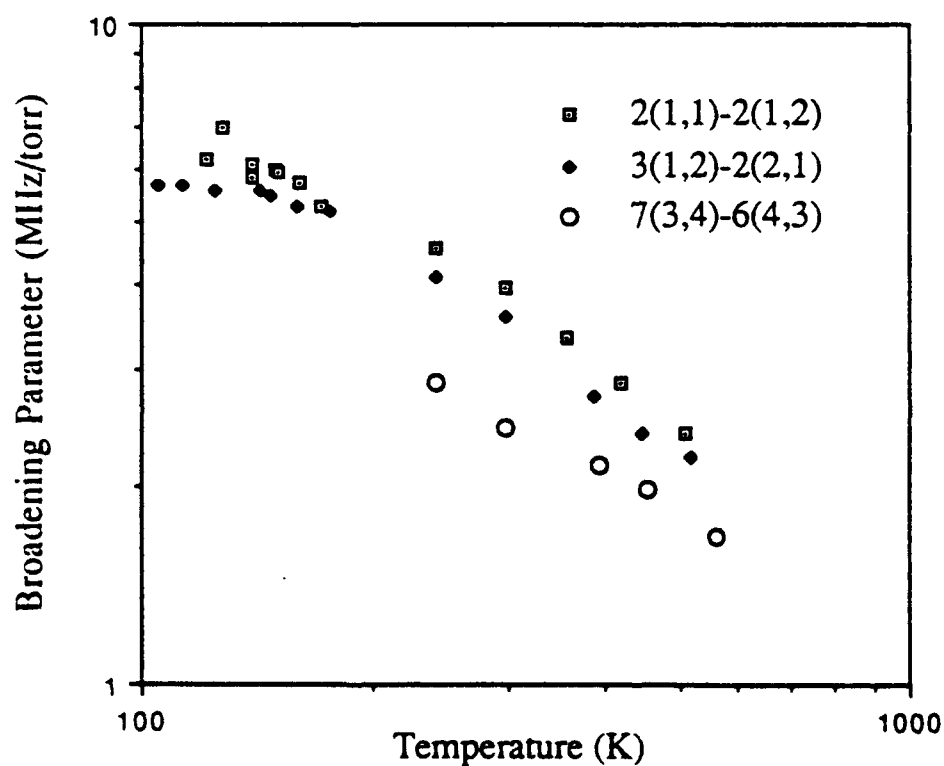
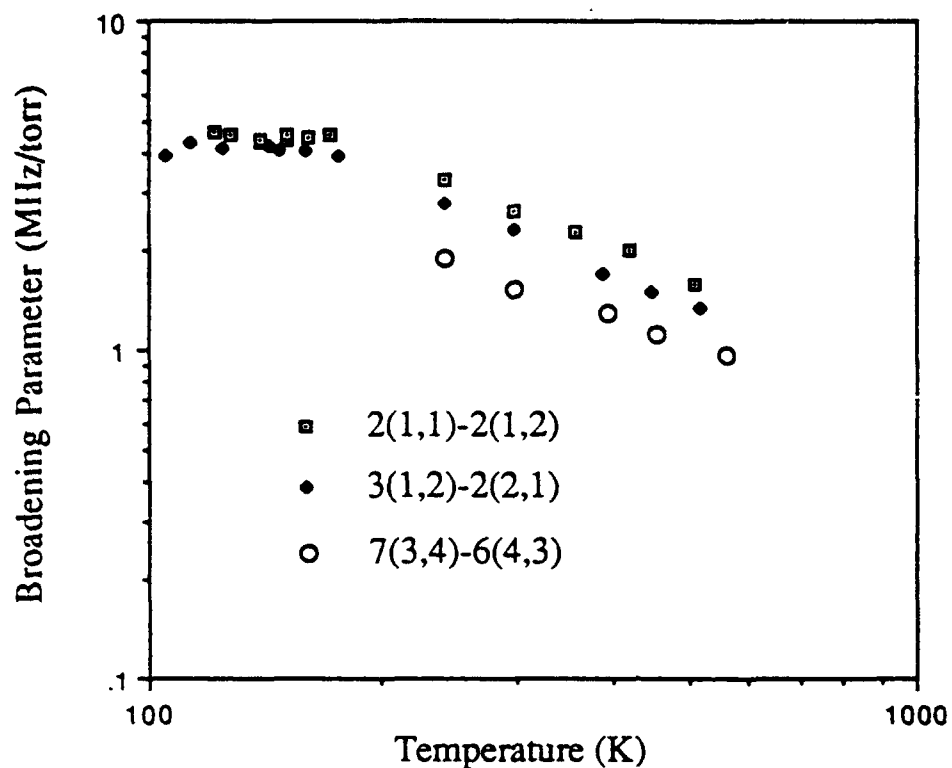


Fig. 3. Measured Pressure Broadening Coefficients Versus Temperature for HDO-He

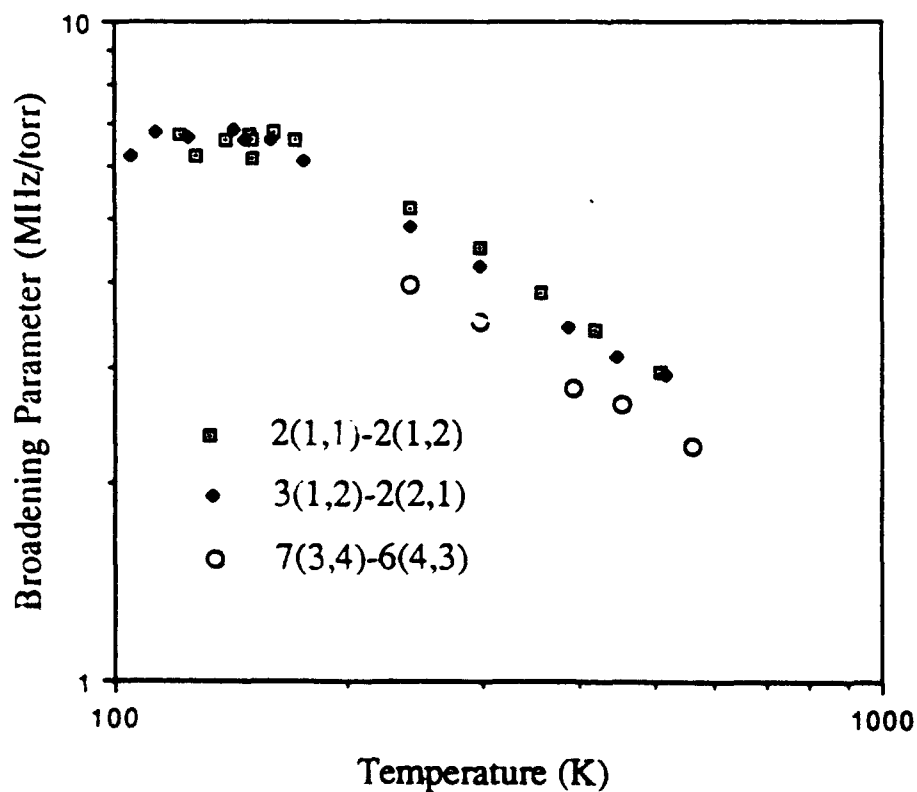
HDO - Hydrogen Broadening

Fig. 4. Measured Pressure Broadening Coefficients Versus Temperature for HDO-H₂

HDO - Oxygen Broadening

Fig. 5. Measured Pressure Broadening Coefficients Versus Temperature for HDO-O₂

HDO - Nitrogen Broadening

Fig. 6. Measured Pressure Broadening Coefficients Versus Temperature for HDO-N₂

Results

The 2(1,1) - 2(1,2) transition of HDO

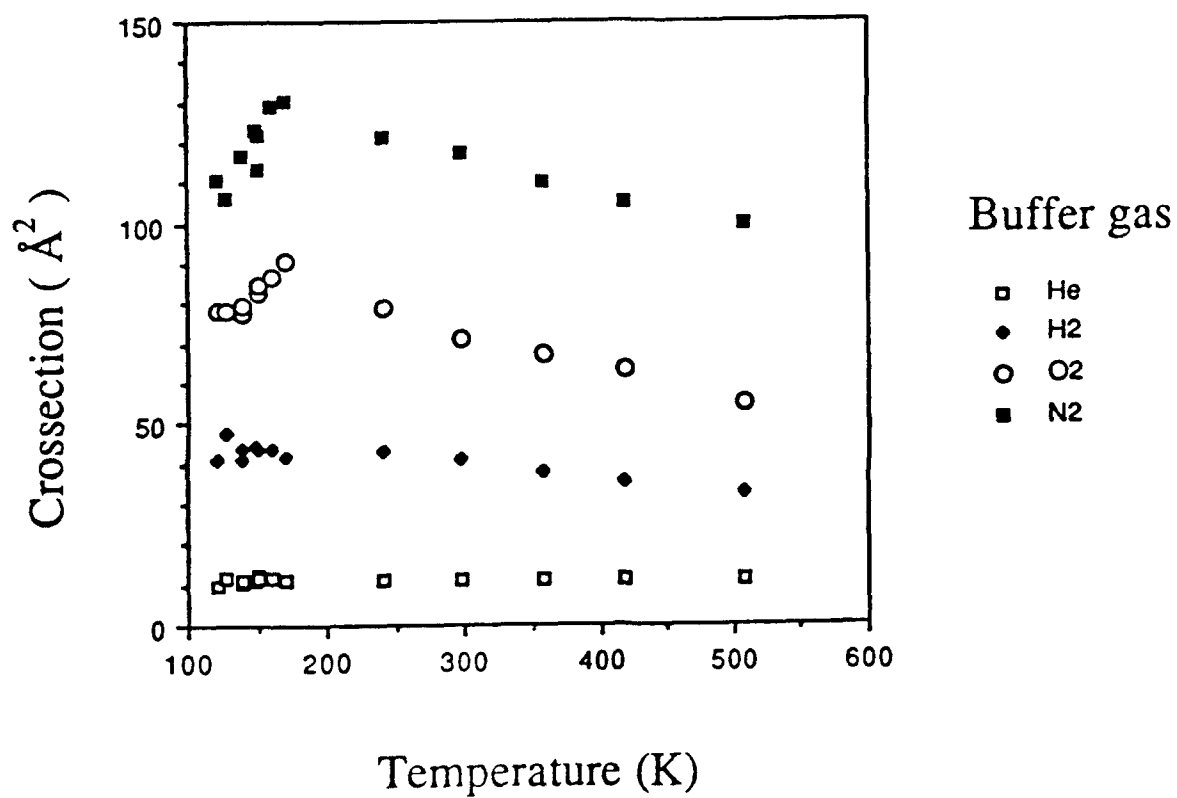


Figure 7.

Results

The 3(1,2) - 2(2,1) transition of HDO

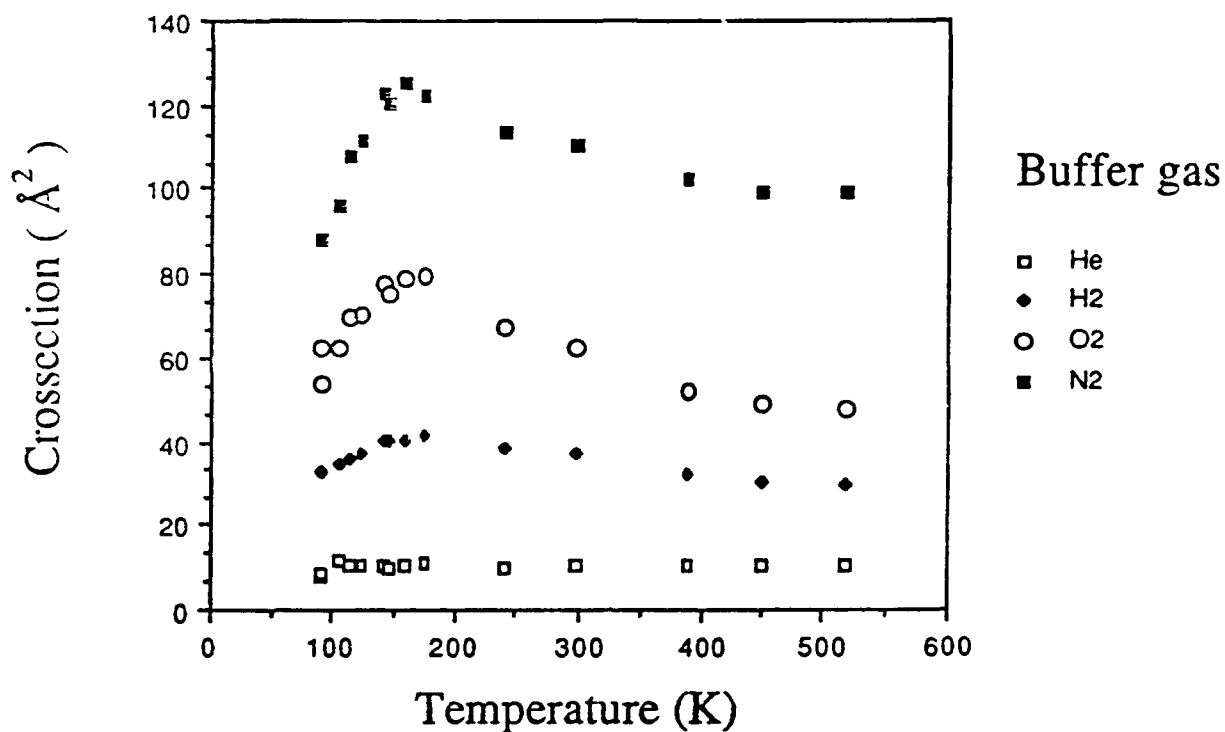


Figure 8.

The 7(3,4) - 6(4,3) transition of HDO

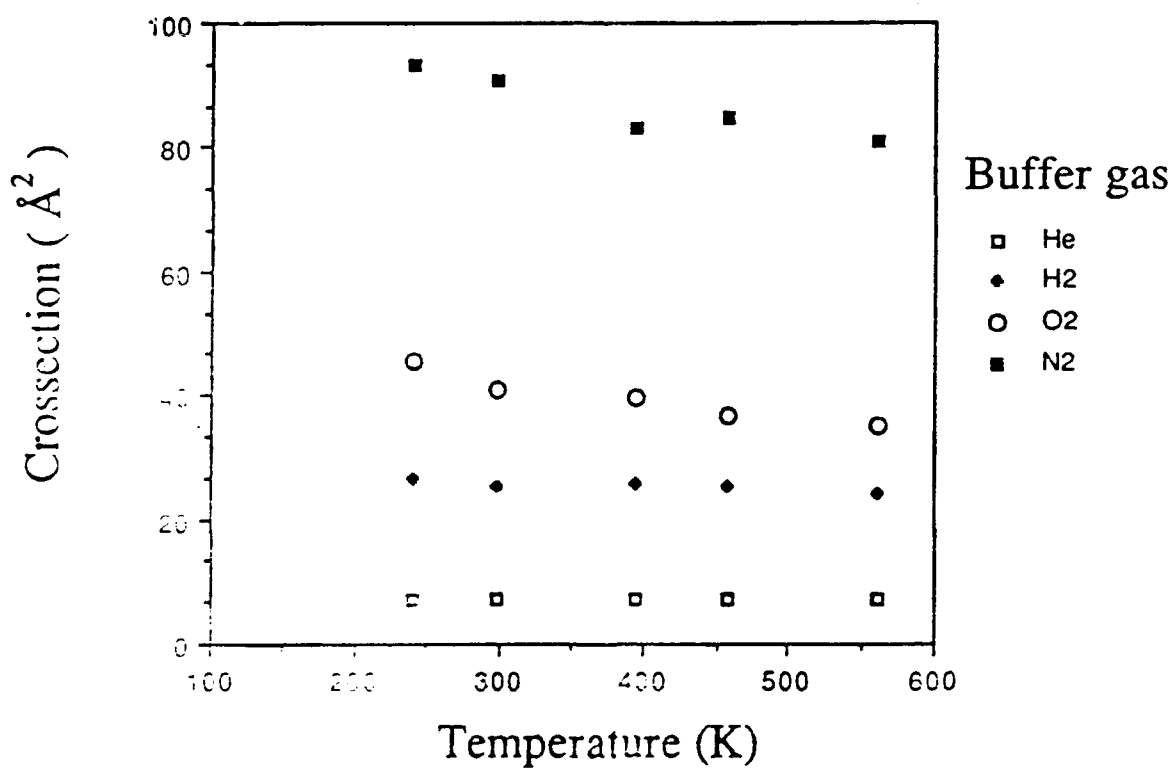


Figure 9.

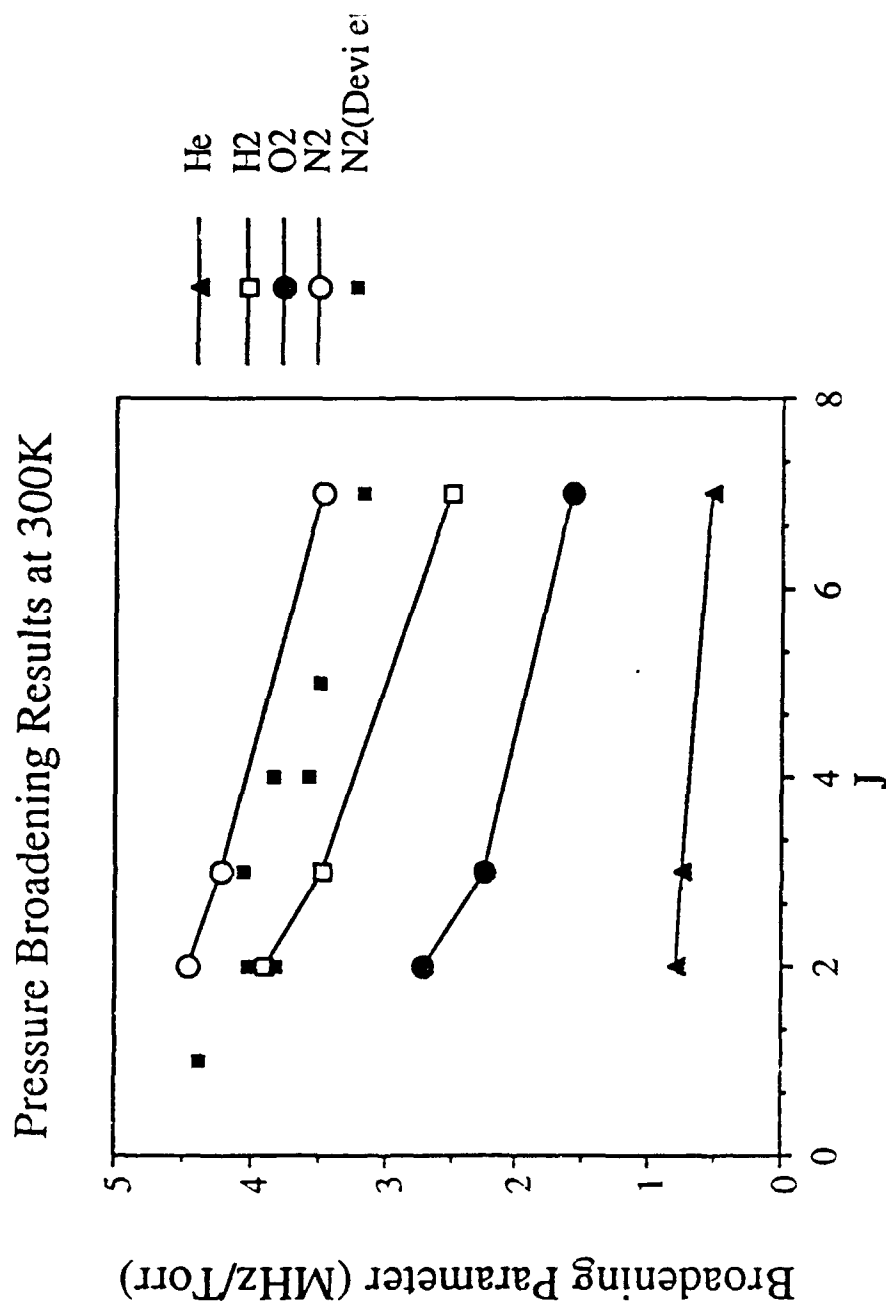


Fig. 10. Pressure Broadening Coefficient at 300K As A Function of Rotational Quantum Number J.

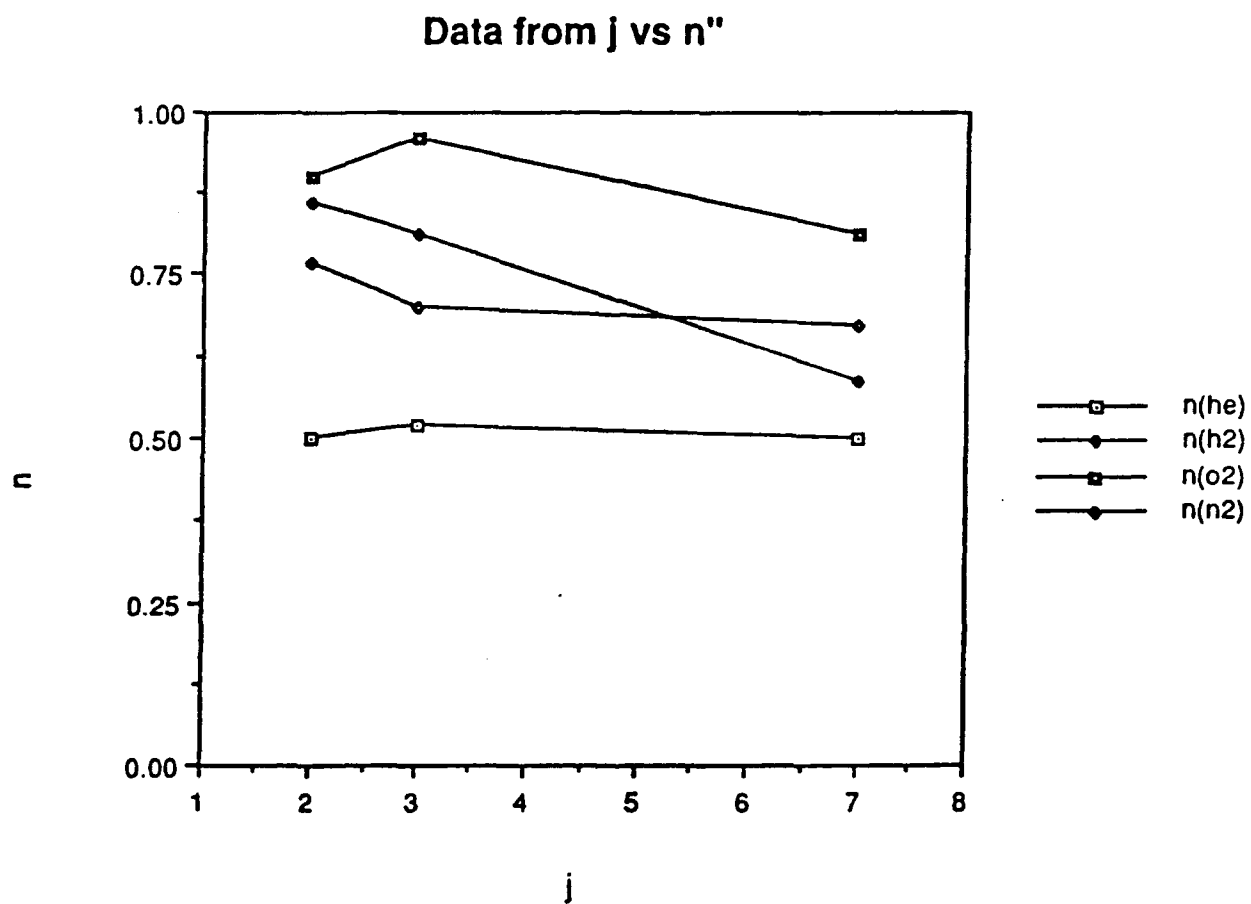


Fig. 11. Temperature Exponent n Versus The Rotational Quantum Number J .